Mean-field calculation including proton-neutron mixing in atomic nuclei —toward proton-neutron pairing—

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◆ “Nuclear DFT (density functional theory) with proton-neutron pairing and its application” (e.g. GT transition in r-process)

- Proton-neutron (p-n) pairing: Goodman, Adv. Nucl. Phys.11, (1979) 293.

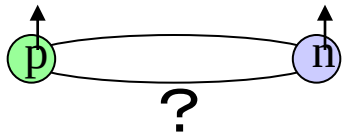
  Pairing between protons and neutrons (isoscalar T=0 and isovector T=1)

  Related (?) physics:

  Wigner energy, β decays , interplay between $T = 0$ and $T = 1$ states in $N = Z$ nuclei, isospin mixing and mirror symmetry breaking, α decay and α clustering, moments of inertia, deformation properties, etc.

  Perlinska et al, PRC 69 , 014316(2004)

  For a review on *p-n* pairing, see A. Afanasjev, arXiv:1205.2134



- Proton-neutron mixing:

  Quasiparticles are mixtures of protons and neutrons

  Density functionals with an arbitrary mixing between protons and neutrons

$$\rho_\tau(\alpha,\beta) = \left\langle \Psi \left| c^+_{\alpha,\tau} c_{\beta,\tau} \right| \Psi \right\rangle \longrightarrow \rho_{\tau\tau'}(\alpha,\beta) = \left\langle \Psi \left| c^+_{\alpha,\tau} c_{\beta,\tau'} \right| \Psi \right\rangle$$

$$\tau = p,n \qquad \tau,\tau' = p,n$$

As a first step, we consider p-n mixing at the Hartree-Fock level without pairing.

Hartree-Fock calculation including proton-neutron mixing

- Extension of the single particle states

$$\left|\psi_{i,n}\right\rangle = \sum_{\alpha} a_{i,\alpha}^{(n)} \left|\alpha, n\right\rangle$$
$$\left|\psi_{j,p}\right\rangle = \sum_{\alpha} a_{j,\alpha}^{(p)} \left|\alpha, p\right\rangle$$

$$\longrightarrow \quad \left|\psi_{i}\right\rangle = \sum_{\alpha} a_{i,\alpha}^{(n)} \left|\alpha, n\right\rangle + \sum_{\beta} a_{i,\beta}^{(p)} \left|\beta, p\right\rangle$$

i=1,…,A

- Extension of the density functional

$$E^{Skyrme}[\rho_n, \rho_p] \longrightarrow E^{Skyrme'}[\rho_0, \vec{\rho}\,]$$

Invariant under rotation in isospin space

isoscalar isovector

Perlinska et al, PRC 69 , 014316(2004)

can be written in terms of ρ_0, ρ_3

not invariant under rotation in isospin space

$$\rho_0 = \rho_n + \rho_p \qquad \rho_1 = \rho_{np} + \rho_{pn}$$
$$\rho_2 = -i\rho_{np} + i\rho_{pn}$$
$$\rho_3 = \rho_n - \rho_p$$

Energy density functional is extended such that it becomes invariant under rotation in isospin space

Hartree-Fock calculation including proton-neutron mixing

- Extension of the single particle states

$$\left|\psi_{i,n}\right\rangle = \sum_{\alpha} a_{i,\alpha}^{(n)} \left|\alpha, n\right\rangle$$
$$\left|\psi_{j,p}\right\rangle = \sum_{\alpha} a_{j,\alpha}^{(p)} \left|\alpha, p\right\rangle$$

$$\longrightarrow \quad \left|\psi_{i}\right\rangle = \sum_{\alpha} a_{i,\alpha}^{(n)} \left|\alpha, n\right\rangle + \sum_{\beta} a_{i,\beta}^{(p)} \left|\beta, p\right\rangle$$

i=1,…,A

- Extension of the density functional

$$E^{Skyrme}[\rho_n, \rho_p] \longrightarrow E^{Skyrme'}[\rho_0, \vec{\rho}\,]$$

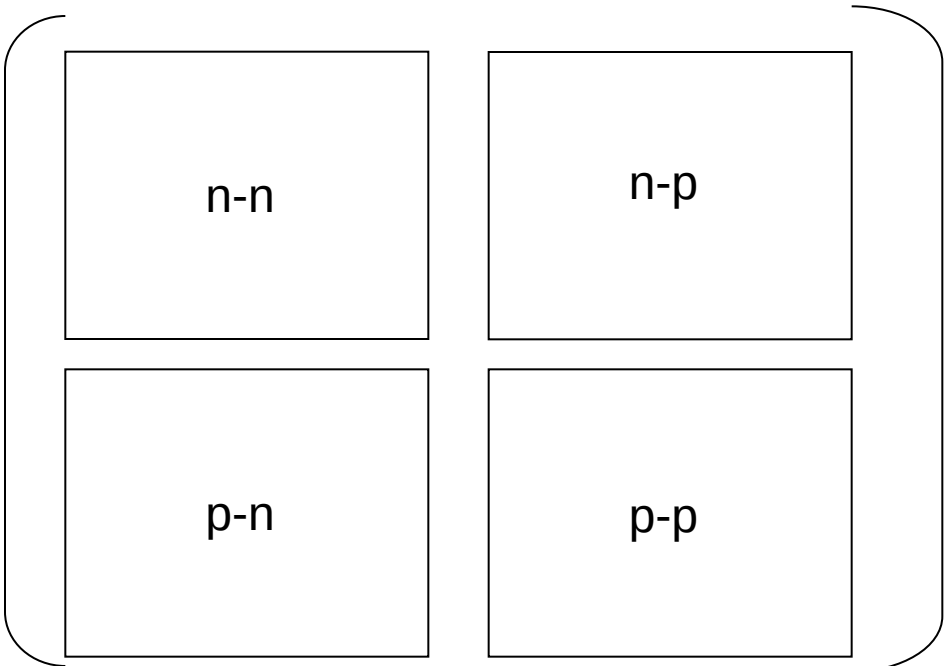
Invariant under rotation in isospace

isoscalar isovector

Perlinska et al, PRC 69 , 014316(2004)

- p-n mixed Hartree-Fock Hamiltonian :

$$h_n, \; h_p \longrightarrow h_{mixed} =$$



Off-diagonal blocks are zero
in the normal HF w/o p-n mixing

It is a hard task to develop a code from scratch …

→ Use of a existing HFB code

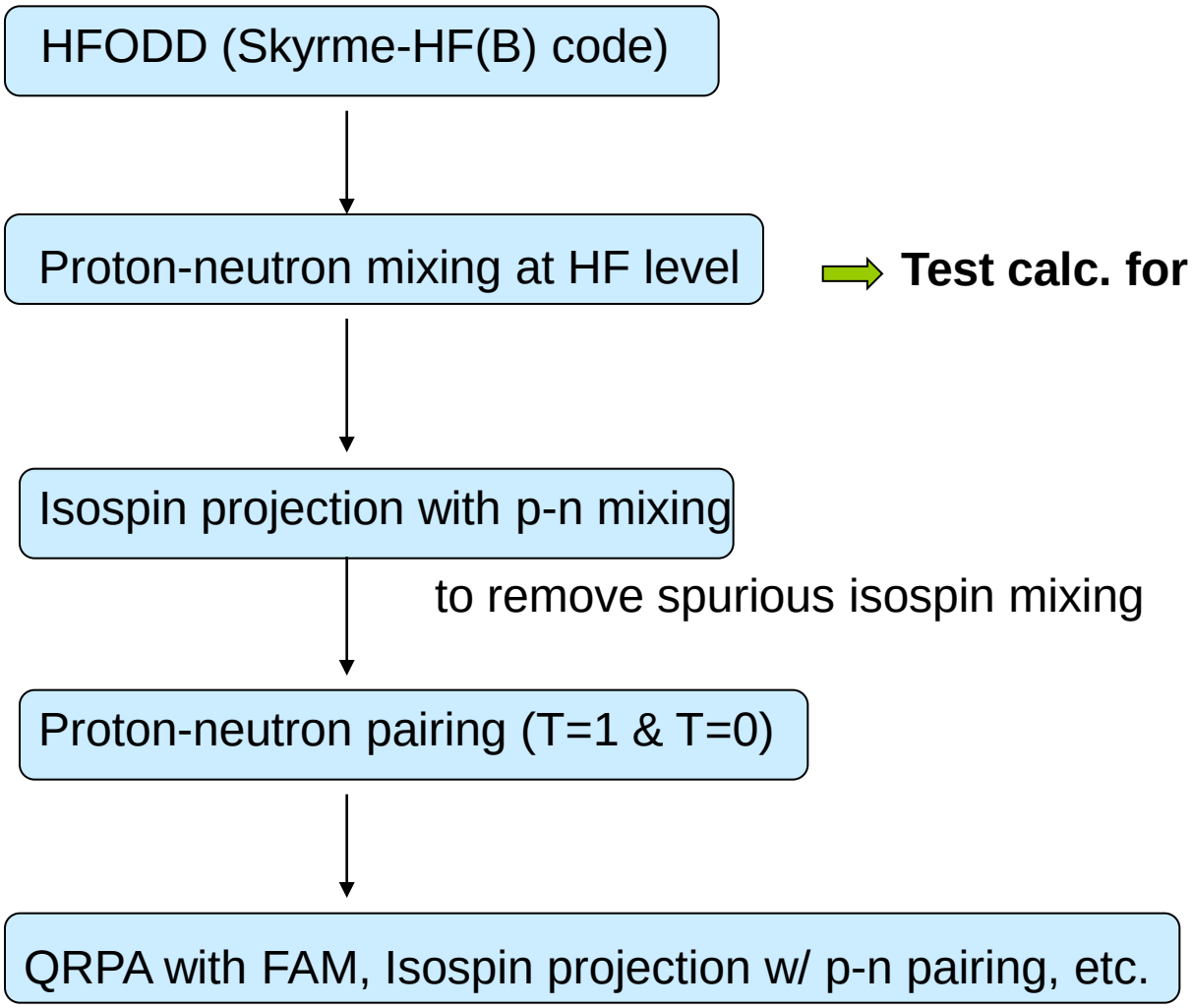
HFODD(1997-)

http://www.fuw.edu.pl/~dobaczew/hfodd/hfodd.html

J. Dobaczewski, J. Dudek, Comp. Phys. Comm 102 (1997) 166.
J. Dobaczewski, J. Dudek, Comp. Phys. Comm. 102 (1997) 183.
J. Dobaczewski, J. Dudek, Comp. Phys. Comm. 131 (2000) 164.
J. Dobaczewski, P. Olbratowski, Comp. Phys. Comm. 158 (2004) 158.
J. Dobaczewski, P. Olbratowski, Comp. Phys. Comm. 167 (2005) 214.
J. Dobaczewski, et al., Comp. Phys. Comm. 180 (2009) 2391.
J. Dobaczewski, et al., Comp. Phys. Comm. 183 (2012) 166.

- Skyrme energy density functional
- Hartree-Fock or Hartree-Fock-Bogoliubov
- No spatial & time-reversal symmetry restriction
- Harmonic-oscillator basis
- Multi-function (constrained HFB, cranking, angular mom. projection, isospin projection, finite temperature….)

Road map

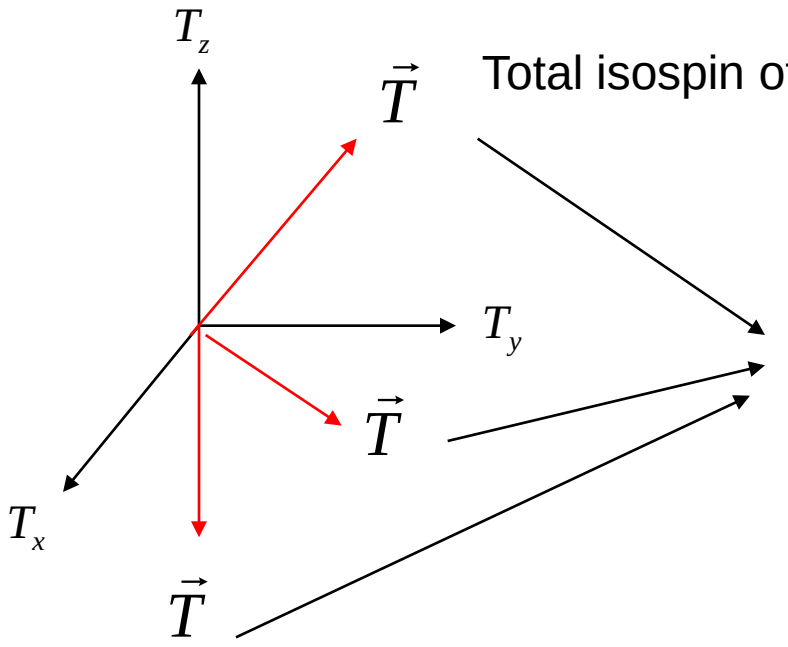

HFODD (Skyrme-HF(B) code)
Proton-neutron mixing at HF level
Test calc. for A=14 and 48 nuclei
Isospin projection with p-n mixing
to remove spurious isospin mixing
Proton-neutron pairing (T=1 & T=0)
QRPA with FAM, Isospin projection w/ p-n pairing, etc.
e.g. calc. of GT strengths of n-rich nuclei

Test calculations for p-n mixing

EDF with p-n mixing is correctly implemented?

w/o Coulomb force (and w/ equal proton and neutron masses)

$\mathcal{H} = \mathcal{H}_{\mathrm{kin}} + \mathcal{H}_{\mathrm{Skyrme}}$:invariant under rotation in isospin space



Total isospin of the system

Rotational invariance in isospace

Total energy should be independent of the orientation of T.

Check of the code

How to control the isospin direction ?

Isocranking calculation

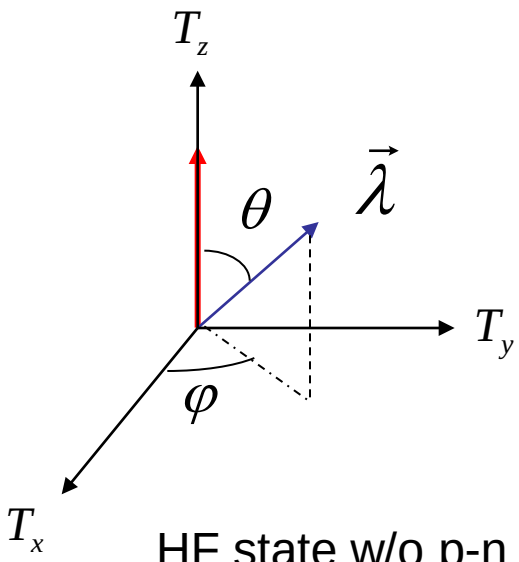
$\hat{H}' = \hat{H} - \vec{\lambda} \cdot \vec{T}$ Isocranking term

$\vec{\lambda}$: Input frequency to control the isospin of the system

HF eq. solved by iterative diagonalization of MF Hamiltonian.

w/ p-n mixing and no Coulomb

Initial state: HF solution w/o p-n mixing (e.g. ^{14}C(Tz=1,T~1))



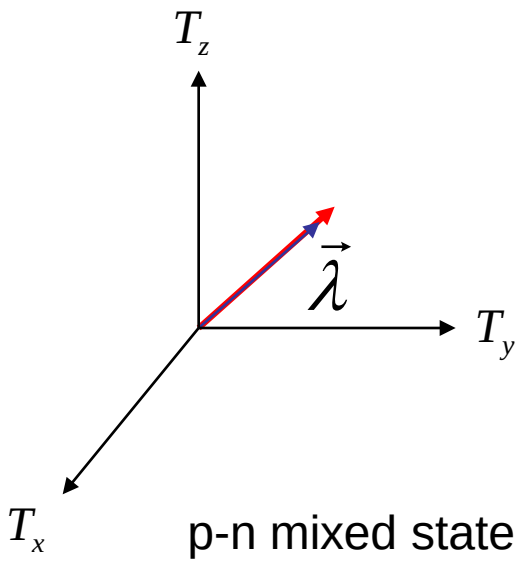
HF state w/o p-n mixing

Determine s. t. proton and neutron Fermi energies become equal

$-\vec{\lambda} \cdot \vec{T}$

iteration

Final state



p-n mixed state

Calculation for A=14 isobars

- w/ p-n mixing and no Coulomb
- w/ p-n mixing and Coulomb

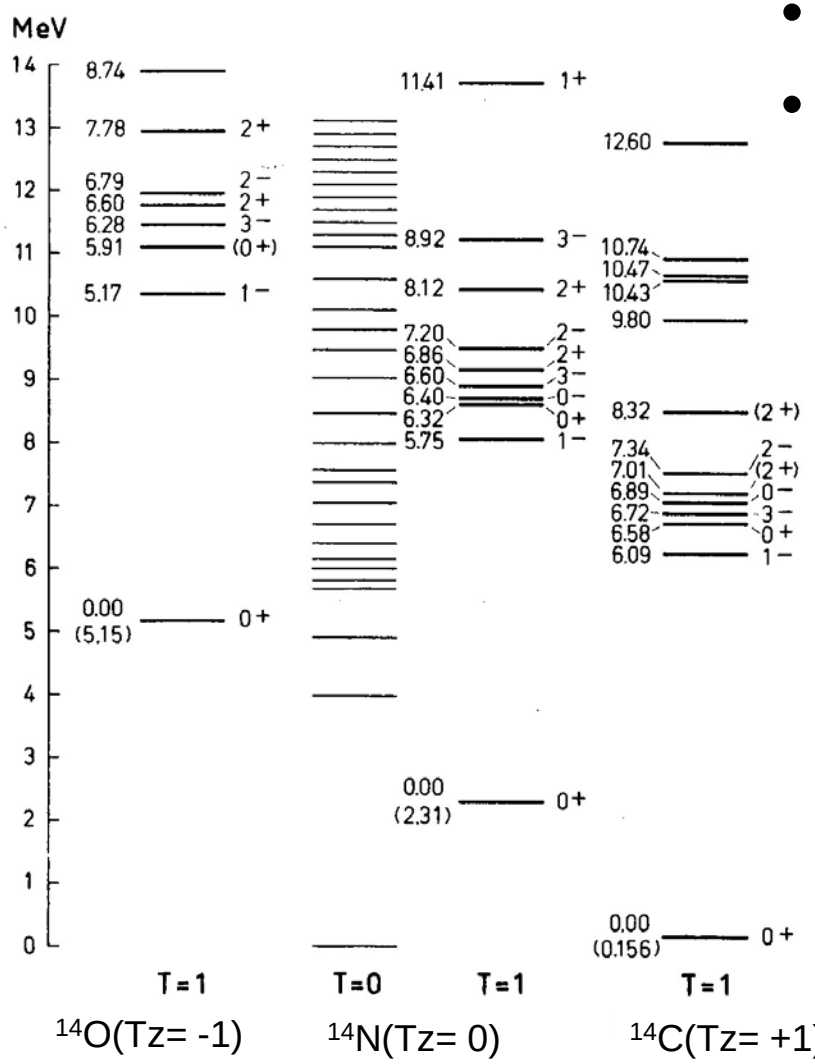
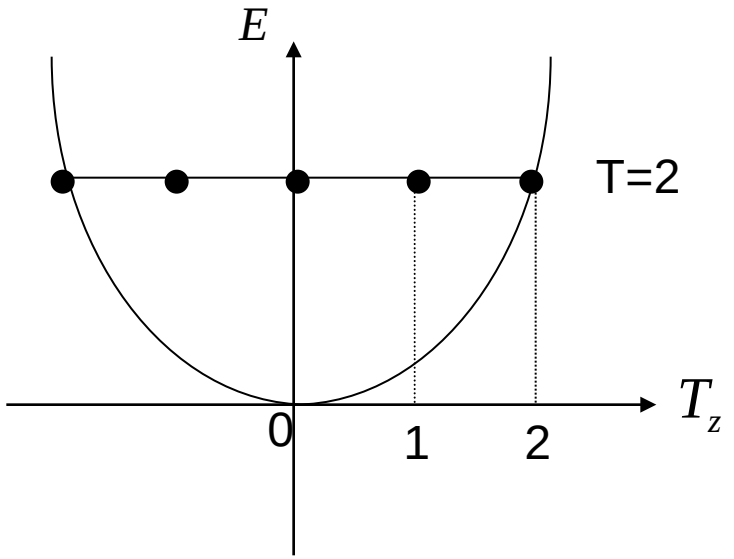


Figure 1-7 The level schemes for the nuclei with $A = 14$ are based on the compilation by F. Ajzenberg-Selove and T. Lauritsen, *Nuclear Phys.* **11**, 1 (1959), on the results given by D. E. Alburger, A. Gallmann, J. B. Nelson, J. T. Sample, and E. K. Warburton, *Phys. Rev.* **148**, 1050 (1966), and on a private communication by G. Ball and J. Cerny (August, 1966). The relative energies represent atomic masses.

Isobaric symmetry



Bohr & Mottelson, “Nuclear Structure” vol.1

Without Coulomb interaction

(Initial : 14C)

^{14}C

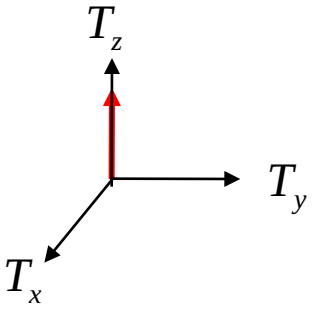
$(\theta,\varphi)=(0,0)$

single-particle energy:

NO)	ENERGY	<T>
1)	-38.419	100
2)	-38.419	100
3)	-32.707	-100
4)	-32.707	-100
5)		
6)		
7)		
8)		
9)		
10)		
11)		
12)		
13)	-15.181	100
14)	-15.181	100

Total energy: -114.611699

$\left\langle \hat{T}_z \right\rangle = 1$



the same s. p energies

$(\theta,\varphi)=(90^\circ,0)$

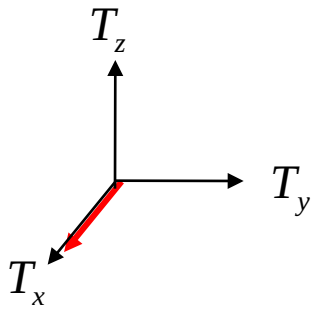
single-particle energy:

NO)	ENERGY	<T>
1)	-38.419	0
2)	-38.419	0
3)	-32.707	0
4)	-32.707	0
5)	-	
6)	-	
7)		
8)		
9)	-	
10)	-	
11)	-	
12)	-	
13)	-15.181	0
14)	-15.181	0

Total energy: -114.611699

$\left\langle \hat{T}_z \right\rangle = 0$

50% neutron &50% proton



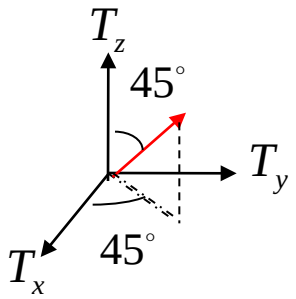
$(\theta,\varphi)=(45^\circ,45^\circ)$

single-particle energy:

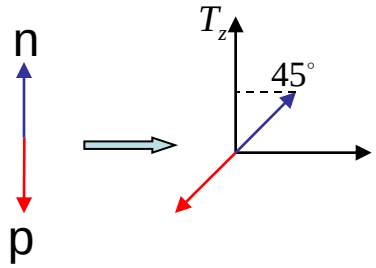
NO)	ENERGY	<T>
1)	-38.419	70.7
2)	-38.419	70.7
3)	32.707	-70.7
4)	-32.707	-70.7
5)		
6)		
7)		
8)		
9)		
10)		
11)		
12)		
13)	-15.181	70.7
14)	-15.181	70.7

Total energy: -114.611699

$\left\langle \hat{T}_z \right\rangle = 0.707$



$\frac{|\vec{\lambda}|}{2} = 5.5$



the same total energies

$\langle T \rangle = \left\langle \frac{1}{2}\tau_z \right\rangle \times 200$

- 100: pure n
- -100: pure p

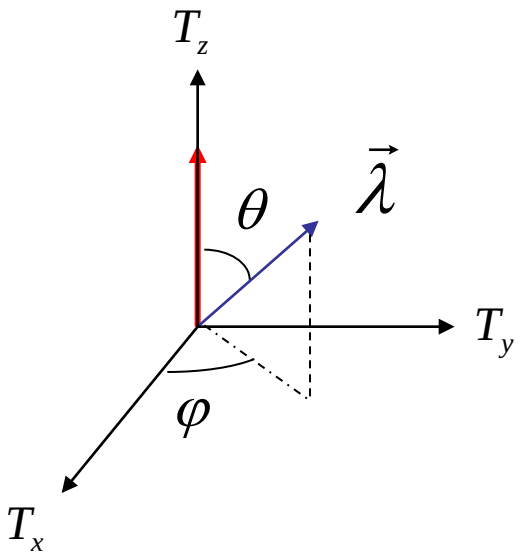
With Coulomb interaction

$U^{Coulomb}(\tau_z)$:violates isospin symmetry

The total energy is now dependent on Tz

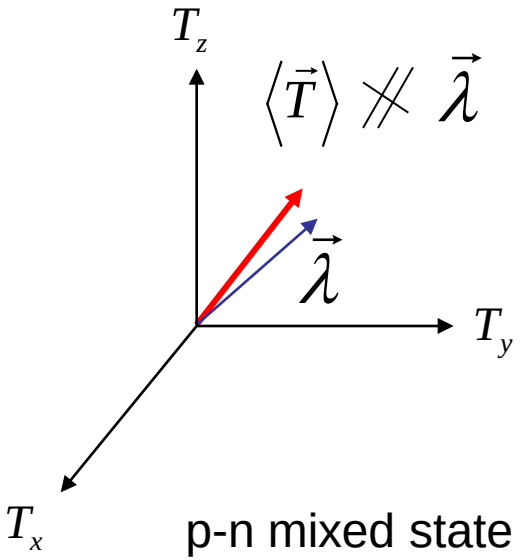
but independent of Tx and Ty

Initial state:



$-\vec{\lambda}\cdot\hat{\vec{T}}$

final state:

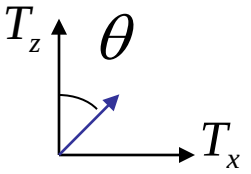


p-n mixed state

HF state w/o p-n mixing

With Coulomb, larger $<T_z>$ is favored

With Coulomb interaction



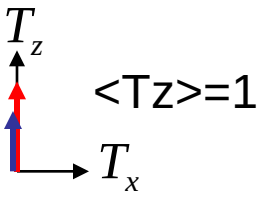
$|\vec{\lambda}| = 11.0\text{MeV}$ $\varphi = 0$

$\theta = 0^\circ$ ⇒ ^{14}C

single-particle energy:

NO)	ENERGY	<T>
1)	-38.346	100
2)	-38.346	100
3)	-29.620	-100
4)	-29.620	-100
5)	-22.000	100
6)	-22.000	100
7)		
8)		
9)	⋮	
10)		
11)		
12)		
13)		
14)		

Total energy: -106.68



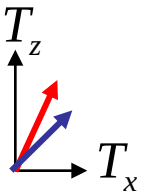
<Tz>=1

$\theta = 45^\circ$

Single-particle energy:

NO)	ENERGY	<T>
1)	-37.980	82.0
2)	-37.980	82.0
3)	-29.880	-82.0
4)	-29.880	-82.0
5)	-21.666	80.7
6)	-21.666	80.7
7)		
8)		
9)	⋮	
10)		
11)		
12)		
13)		
14)		

Total energy: -106.16



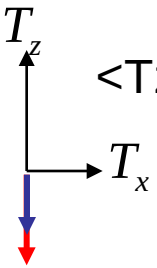
<Tz>=0.802

$\theta = 180^\circ$ ⇒ ^{14}O

single-particle energy:

NO)	ENERGY	<T>
1)	-34.362	-100
2)	-34.362	-100
3)	-32.527	100
4)	-32.527	100
5)	-18.41	-100
6)	-18.41	-100
7)	.	
8)	.	
9)	.	⋮
10)	.	
11)	-	
12)	.	
13)	.	
14)	.	

Total energy: -100.70

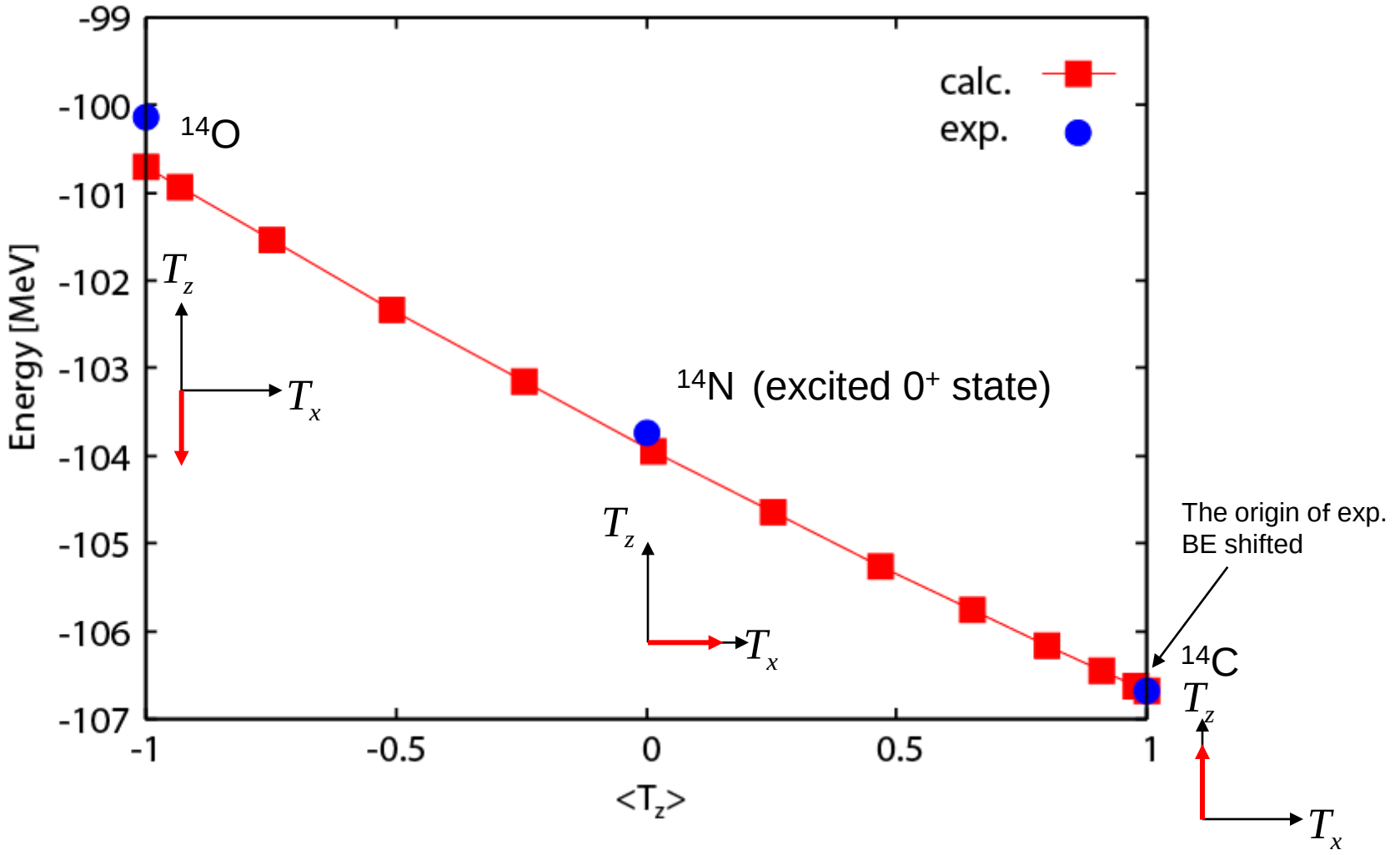


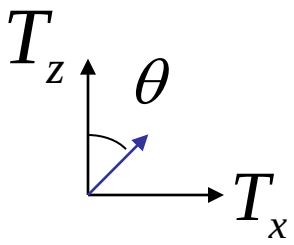
<Tz>=-1

- Total and s. p. energies depend on <Tz>
- Total isospin and $\vec{\lambda}$ are not parallel for p-n mixed states
- No p-n mixing for $\theta = 0^\circ$ and $\theta = 180^\circ$

(Neither Coulomb nor isocranking term contains Tx and Ty.)

Tz dep. of the total energy and comparison with data



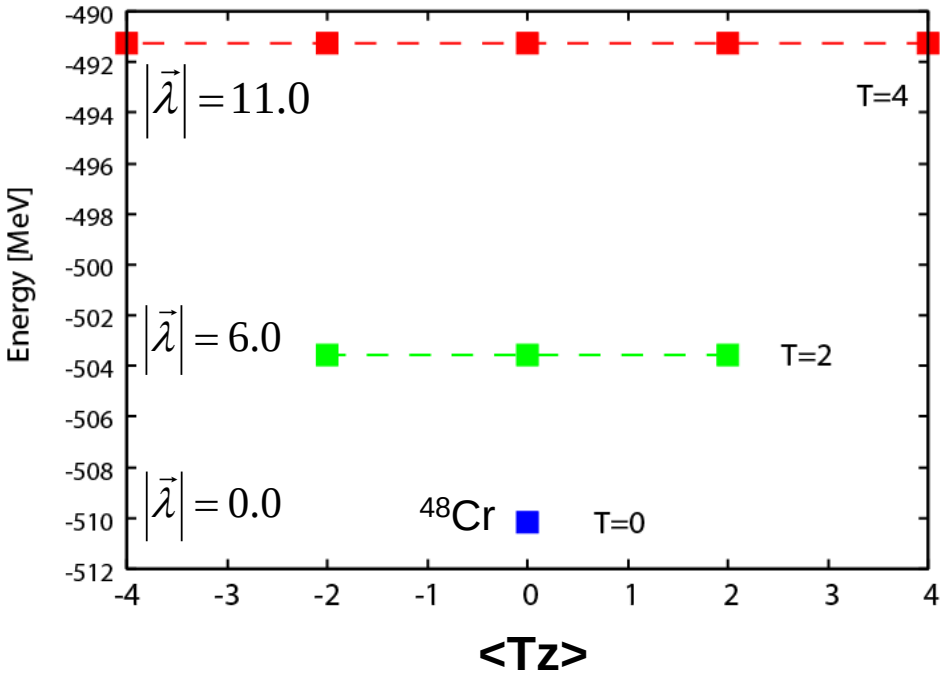


exp.: binding energy
(+excitation energy for 14N)

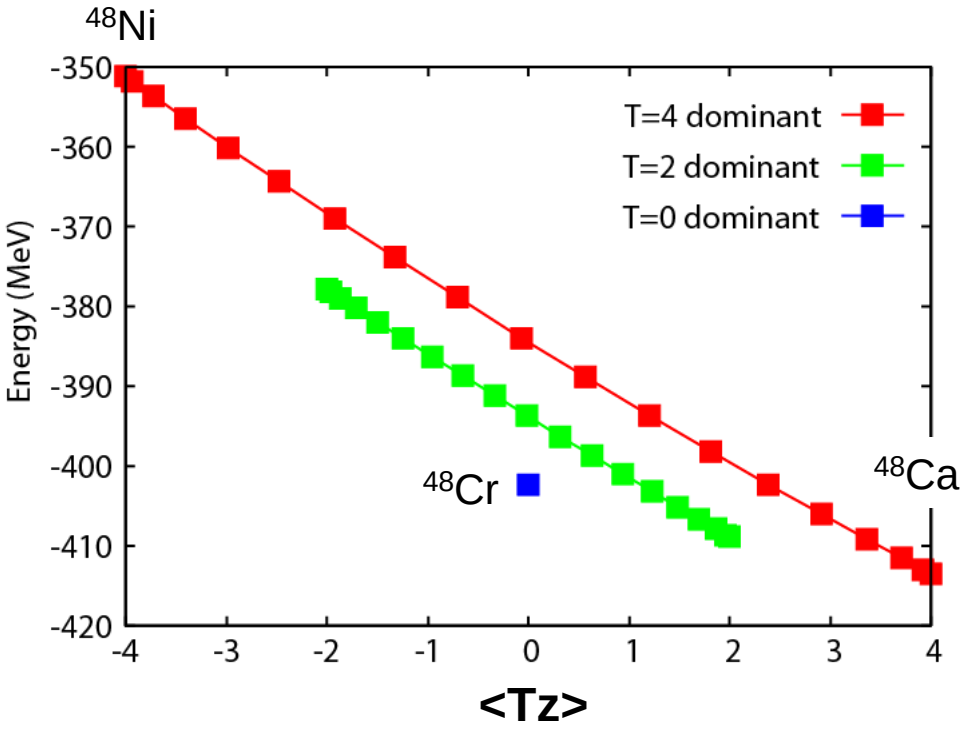
calc.: calculated for
every 15° of θ from 0 to 180°

Result for A=48 isobars

Initial : 48Cr(Tz=0, T~0)



Without Coulomb



With Coulomb

Without Coulomb

- Increase the size of isofrequency $|\vec{\lambda}|$ to make high-isospin states

With Coulomb

- Tune the size of lambda depending on the tilting angle θ
- Diabatic blocking with isospin to avoid oscillatory (ping-pong) divergence

J. Dobaczewski, J. Dudek, Comp. Phys. Comm. 131 (2000) 164.

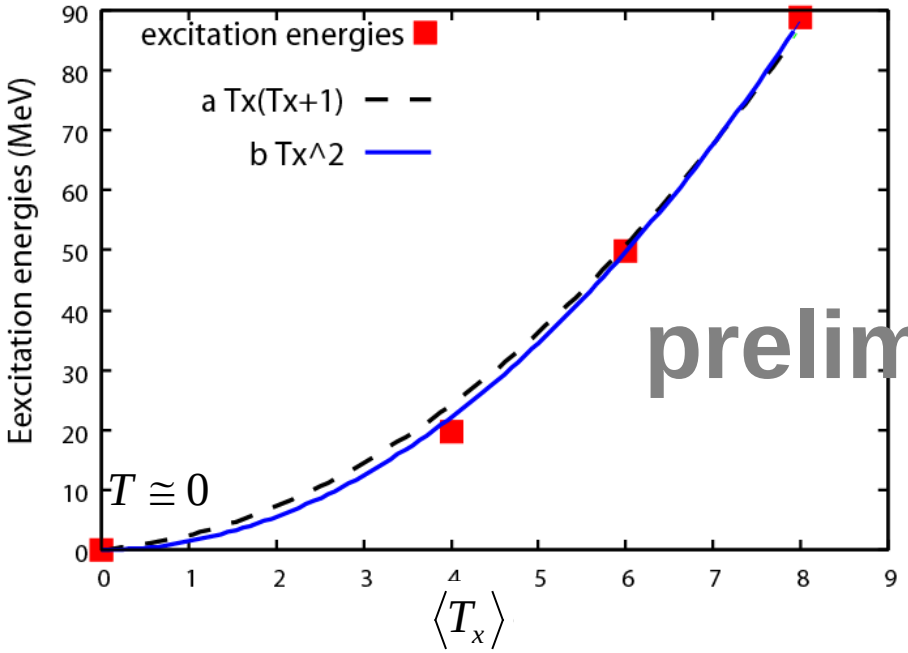
Constrained HF with Augmented Lagrange method

$$E' = E - \vec{\lambda}\cdot\hat{\vec{T}} + C\left(\hat{\vec{T}} - \bar{\vec{T}}\right)^2$$

A. Staszczak, Eur. Phys. J. A **46**, 85–90 (2010)

Excitation energies for 48Cr(Tz=0)

constraints Tz=0 and Tx=0,2,4,6,…



--> nuclear symmetry energy

preliminary

a=1.20956 (MeV)
b=1.38078 (MeV)

Sum of squared residuals :

a*Tx*(Tx+1) fit : 24.2
b*Tx^2 fit : 6.1

$\bar{T}_x$	$\lvert\langle\hat{T}_x\rangle - \bar{T}_x\rvert$	$\bar{T}_z$	$\lvert\langle\hat{T}_z\rangle - \bar{T}_z\rvert$	Energy
2		0		Not yet
4	3.6E-05	0	<1.0E-08	-390.06
6	9.8E-04	0	5.7E-06	-359.76
8	9.4E-04	0	3.1E-06	-320.89

Summary

We have developed a code for the DFT calculations with

- ✔ proton-neutron mixing at the Hartree-Fock level
- ✔ diabatic blocking method using isospin
- ✔ constraints on isospin with augmented Lagrange method

and performed test calculations for A=14 & 48 systems

Ongoing

- ◇ Isospin projection to remove spurious isospin mixing

W. Satuła et al., PRC 81, 054310 (2010).

Future

- ◇ Proton-neutron pairing (T=0 & T=1; non-rotating & rotating)
- ◇ Charge exchange reaction in neutron-rich nuclei (QRPA calculation)

⟶ A very wide applicability expected